

Multiplicity of Generation, Selection, and Classification Procedures for Jammed Hard-Particle Packings

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Abstract

Hard-particle packings have served as useful starting points to study the structure of diverse systems such as liquids, living cells, granular media, glasses, and amorphous solids. Howard Reiss has played a major role in helping to illuminate our understanding of hard-particle systems, which still offer scientists many interesting conundrums. Jammed configurations of hard particles are of great fundamental and practical interest. What one precisely means by a “jammed” configuration is quite subtle and considerable ambiguity remains in the literature on this question. We will show that there is a multiplicity of generation, selection, and classification procedures for jammed configurations of identical d -dimensional spheres. We categorize common ordered lattices according to our definitions and discuss implications for random disk and sphere packings. We also show how the concept of rigidity percolation (which has been used to understand the mechanical properties of network glasses) can be generalized to further characterize hard-sphere packings.

1 Introduction

The problem of packing particles into a container or vessel of some type is one of the oldest problems known to man. Bernal¹ has remarked that “heaps (close-packed arrangements of particles) were the first things that were ever measured in the form of basketfuls of grain for the purpose of trading or the collection of taxes.” Today scientists study particle packings in order to understand the structure of living cells, liquids, granular media, glasses and amorphous solids, to mention but a few examples. Since the structure of such systems is primarily determined by the repulsive interactions between the particles, the hard-sphere model serves as a useful idealized starting point for such an investigation.^{2–6}

Hard spheres interact with each other only when they touch, and then with an infinite repulsion reflecting their impenetrable physical volume. Despite the simplicity of the hard-sphere potential, hard-sphere systems offer many conundrums, several of which we will briefly describe. The first example concerns the existence of an entropically driven disorder/order phase transition in hard-sphere and hard-disk (two-dimensional) systems. Although there is strong numerical evidence to support the existence of a first-order disorder/order phase transition in three dimensions, a rigorous proof for such a transformation is not yet available. In two dimensions, the state of affairs is even less certain because it is not clear (from numerical simulations) whether the transition, if it exists, is first-order or a continuous Kosterlitz–Thouless–Halperin–Nelson–Young (KTHNY) transformation.^{7–9}

Another conundrum involves the determination of the densest packing of identical hard spheres. It is only recently that a putative air-tight rigorous proof has been devised for Kepler’s conjecture: the densest possible packing fraction ϕ for identical spheres in three dimensions is $\pi/\sqrt{18} \approx 0.7405$, corresponding to the close-packed face-centered cubic (FCC) lattice or its stacking variants.¹⁰ Although the neighborhood grocer would have given the same solution, proving Kepler’s conjecture is another matter. The difficulty arises because the densest local packing is inconsistent with global packing constraints, i.e., nonoverlapping regular tetrahedra cannot tile space. This is not true in two dimensions, where the densest local packing is consistent with the densest global packing.

Yet another example of a conundrum concerns the venerable notion of “random close packing” (RCP) of hard spheres. The traditional notion of the RCP state is that it is the maximum density that a large, irregular arrangement of spheres can attain and that this density is a well-defined and unique quantity. It was recently shown that the RCP state is in fact mathematically ill-defined and must be replaced by a new notion called the *maximally random jammed* (MRJ) state, which can be made precise.¹¹ The identification of the MRJ state rests on the development of metrics for order (or disorder), a very challenging problem in condensed-matter theory, and a precise definition for the term “jammed.” Torquato et al.¹¹ have suggested and computed several scalar metrics for order in hard-sphere systems and have introduced a precise definition of “jammed.” This formalism provides a means of classifying jammed structures in terms of their degree of order in an “ordering” phase diagram¹. For example, let ψ represent a scalar order metric that varies between unity in the case of perfect order and zero in the case of perfect disorder, and imagine the set of all jammed structures in the ϕ - ψ plane. The MRJ state is simply the configuration of particles that minimizes ψ (maximizes the disorder) among all statistically homogeneous and isotropic *jammed* structures. More generally, the identification of the boundaries of the set of all jammed structures is a problem of great interest. Besides the MRJ state, for example, one may wish to know the lowest density jammed structure(s), which is an open problem in two and three dimensions. We also note that the concept of a jammed structure is particularly relevant to the flow, or lack thereof, of granular media.^{12,13}

In this paper, we will focus our attention on the question, What does one really mean by a “jammed” hard-particle system? The answer to this question is quite subtle and a failure to appreciate the nuances involved has resulted in considerable ambiguity in the literature on this question. Yet a precise definition for the term “jammed” is a necessary first step before one can undertake a search for jammed structures in a meaningful way. We will show that there is a multiplicity of definitions for jammed structures. For simplicity and definiteness, we will restrict ourselves to equi-sized d -dimensional hard spheres in d -dimensional Euclidean

¹Perhaps more importantly, the ordering phase diagram can also serve as a means for mapping the degree of order in nonequilibrium (or history-dependent) structures as a function of their processing conditions.

space. Of particular concern will be the cases of equi-sized hard circular disks ($d = 2$) and equi-sized hard spheres ($d = 3$).

2 Definitions

We will consider N equi-sized d -dimensional hard spheres of diameter D . To begin, we will assume that the N particles are confined to a convex region of d -dimensional Euclidean space of volume V with impenetrable but possibly deformable boundaries. The boundaries are assumed to be smooth on the scale of the particle diameter. Periodic boundary conditions will be mentioned separately below.

A particle in the system is individually jammed if it cannot be translated while holding fixed the positions of all of the other $N - 1$ particles in the system. This means that a particle in the bulk must have at least $d + 1$ neighbor or wall contacts not all of which are in the same “hemisphere.” A necessary condition for the entire system to be jammed is that each of the N particles is individually jammed. The system of disks shown in Fig. 1 meets this necessary condition, but all are in contact with the impenetrable boundary, and consequently leave the interior of the system entirely vacant. Analogous three-dimensional examples can also be identified, with all spheres jammed against the boundary, leaving the interior of the system totally unoccupied. While such unusual cases may have some intrinsic interest, we leave them aside for present purposes by requiring that at least one particle of the jammed configuration not contact the boundary. This leaves open the possibility that the interior of some disk and sphere packings might display relatively large voids or cavities surrounded by a “cage” of jammed particles.

Note that these minimal requirements mean that there can be no “rattlers” (i.e., movable but caged particles) in the system. It should be recognized that jammed structures created in practice via computer algorithms¹⁴ or actual experiments may contain a small concentration of such rattler particles, the precise concentration of which is protocol-dependent. Nevertheless, it is the overwhelming majority of spheres that compose the underlying “jammed” network that confers “rigidity” to the particle packing and, in any case, the “rattlers” could

be removed without disrupting the jammed remainder.

We are now in a position to state our definitions of jammed configurations. A system of N spheres is said to be a

1. *Locally jammed configuration* if the system boundaries are nondeformable and each of the N particles is individually jammed, i.e., it meets the aforementioned necessary condition.
2. *Collectively jammed configuration* if the system boundaries are nondeformable and it is a locally jammed configuration in which there can be no collective motion of any contacting subset of particles that leads to unjamming.
3. *Strictly jammed configuration* if it is collectively jammed and the configuration remains fixed under infinitesimal virtual global deformations of the boundaries. In other words, no global boundary-shape change accompanied by collective particle motions can exist, that respects the nonoverlap conditions.

We emphasize that our definitions do not exhaust the universe of possible distinctions, but they appear to span the reasonable spectrum of possibilities. It is clear that the second definition is more restrictive than the first and the third definition is the most restrictive. It is crucial to observe that the above classification scheme is dependent on the type of boundary conditions imposed (e.g., impenetrable or periodic boundary conditions) as well as the shape of the boundary.

The collectively jammed definition was the one used by Torquato et al.¹¹ in their work on the maximally random jammed state. Note that overall rotation of configurations in a circular or spherical boundary can still leave the system collectively jammed (see, for example, Fig. 1).

Observe that the most restrictive definition of a jammed structure, the *strictly jammed configuration*, is a purely kinematic one, i.e., we do not appeal to a description of forces or stresses on the system. However, one could choose to relate the concomitant stresses on the boundaries to the deformations via some appropriate constitutive relation. For exam-

ple, in the case that the stresses are linearly related to the strains, Hooke's law for linear elasticity would apply and the system would be characterized generally by 21 elastic moduli in three dimensions. In the case of an elastically isotropic packing, two elastic moduli would characterize the system: the bulk modulus K , relating isotropic compressive stresses to corresponding volumetric strains (deformations), and the shear modulus G , relating shear stresses to corresponding volume-preserving strains. Thus, in this latter instance, a strictly jammed configuration is characterized by infinite bulk and shear moduli.

An interesting characteristic of a jammed packing of spheres that has not been studied to our knowledge is its “*rigidity percolation threshold*.” Rigidity percolation has been studied on lattice networks to understand the mechanical properties of network glasses, for example.^{15–17} Consider a triangular net of mass points connected by nearest-neighbor central forces. The system is stable and elastically isotropic, and therefore is characterized by the elastic moduli K and G . If bonds are randomly removed with probability $1 - p$, then both K and G vanish at some critical value p^* between 0 and 1 called the rigidity percolation threshold.

The notion of rigidity percolation can be extended to describe jammed sphere packings. Importantly, in doing so, we do not have to appeal to notions of elasticity. Consider a jammed system that meets one of the three aforementioned definitions. Begin a process whereby spheres are sequentially removed by some selection process with a random element. The rigidity percolation threshold is the sphere volume fraction ϕ^* at which the system ceases to be jammed according to one of our three definitions. Thus, the value of ϕ^* will generally vary for a given structure depending on what is meant by a jammed configuration. For example, for an initial lattice at packing fraction ϕ , the value of ϕ^* will increase as the jamming criterion changes from the least restrictive (locally jammed) to the most restrictive (strictly jammed). In general, ϕ^* must lie in the interval $(0, \phi]$. We believe that this generalization of rigidity percolation will be especially useful in characterizing random jammed packings.

Boundary conditions play an essential role in packing problems. Although the principal focus of the present exposition concerns the case of impenetrable boundaries (on account of their physical significance), we recognize that periodic boundary conditions are often applied in a wide range of many-particle theories and numerical simulations. Note that in the present

context periodic boundary conditions are substantially less confining than are impenetrable-wall boundary conditions, when either could be applied to a given finite particle packing. Hence, the classification scheme defined above may have an outcome that hinges sensitively upon which of these alternatives applies. The simple cubic lattice offers an example; it is collectively jammed with rigid walls, but only locally jammed with periodic boundary conditions.

3 Classification of Some Ordered Lattice Packings

In this section we categorize some common two- and three-dimensional lattice packings according to whether they are locally jammed, collectively jammed, or strictly jammed. In all cases we assume impenetrable but possibly deformable system boundaries. We begin with two-dimensional lattices within commensurate rectangular boundaries. The three-fold coordination of a honeycomb (hexagonal) lattice is sufficient to make this structure locally jammed (see Fig. 2a). Note that the graph that results by drawing lines between nearest-neighbor centers is a hexagonal tiling of the plane for an infinite system. In the infinite-volume limit, the packing fraction $\phi = \pi/(3\sqrt{3}) \approx 0.605$. However, the honeycomb lattice is not collectively jammed, since an appropriate collective rotation of six particles that are situated on the sites of any of the hexagons in the bulk will destabilize the structure. Thus, the honeycomb lattice is also not strictly jammed. Note that by an appropriate placement of three circular disks of diameter $\sqrt{3}D/4$ in each of the original disks of diameter D in Fig. 2a, the packing that results upon removal of the larger disks is locally jammed at the packing fraction $\phi = 3\pi/(4\sqrt{3}) \approx 0.340$ in the infinite-volume limit (see Fig. 2b).

The square lattice is both locally and collectively jammed, but it is not strictly jammed, since a shear deformation (not an isotropic deformation) will destabilize the packing. The Kagomé lattice is not locally jammed in a rectangular container because certain particles along the vertical walls may be moved, leading to an instability (see Fig. 3). However, the Kagomé lattice becomes strictly jammed if it is appropriately situated within a container with either regular triangular- or hexagonal-shaped boundaries. Note that for an infinitely

large system, it has a packing fraction of $\phi = 3\pi/(8\sqrt{3}) \approx 0.680$. The triangular lattice is strictly jammed. It has a packing fraction of $\phi = \pi/\sqrt{12} \approx 0.907$. The classification of all of the aforementioned lattices is summarized in Table 1. An example of a two-dimensional collectively jammed lattice with an appreciably lower packing fraction than the triangular lattice is shown in Fig. 4. This four-coordinated lattice, built from the triangular lattice with one-fourth of the disks missing, was considered by Lubachevsky, Stillinger, and Pinson.¹⁸

Now let us consider some three-dimensional lattices within a cubical container. The tetrahedrally coordinated diamond lattice is the three-dimensional analogue of the honeycomb lattice. It is locally jammed, but is not collectively jammed, and therefore not strictly jammed. The simple cubic lattice is the three-dimensional analogue of the square lattice; it is both locally and collectively jammed, but it is not strictly jammed, since a shear deformation (not an isotropic deformation) in the (100) planes will destabilize the packing. The same characterization is true for the body-centered cubic (BCC) lattice as for the simple-cubic lattice. The BCC lattice is not strictly jammed because a shear deformation in the (110) planes will destabilize the packing. The face-centered cubic lattice is strictly jammed. The hexagonal close-packed lattice is strictly jammed if the container boundary is a hexagonal prism but it is only locally jammed for a cubical boundary.

4 Discussion and Future Work

Let us now turn our attention to the practical determination of our three different definitions for jammed configurations. It is clear that the criteria for a locally jammed configuration will be the easiest to implement in a computer simulation. In two dimensions, one must determine whether each disk is locally jammed, i.e., whether each disk has at least three contacting neighbors that do not all lie in a semicircle surrounding the particle of concern. In three dimensions, one must ascertain whether each sphere has at least four contacting neighbors that do not all lie in a hemisphere surrounding the particle. Error enters the search algorithm because one must choose an acceptable tolerance for the nearest-neighbor distance to determine whether a neighbor is indeed in contact with the reference particle.

The determination of whether the system is collectively jammed is considerably more difficult, especially for a random system. An approximate means to test that the system is collectively jammed is to shrink the particle sizes uniformly by a very small amount, give the particles some random initial velocities, and follow the system dynamics using a molecular dynamics simulation technique. If the particle configuration effectively does not change after a sufficiently long period of time, the system can be regarded to be collectively jammed. This procedure has been used by Lubachevsky, Stillinger, and Pinson¹⁸ to ascertain whether their particle systems were “stable.” Such a stochastic approach is intended to discover if the particle configuration considered contains polygons of contacting neighbors whose simultaneous displacements initiate local unjamming. A desirable objective for future research is the design of a more efficient discovery procedure for these multiparticle unjamming motions.

Interestingly, the determination of whether a particle packing is strictly jammed may be relatively straightforward given that it is collectively jammed. The basic idea is to transform the collectively jammed particle packing into an equivalent Delaunay graph or network. Roughly speaking, the Delaunay network is the polyhedral graph that results by drawing lines between nearest-neighbor centers in the packing.¹⁹ Once this equivalent network is determined, one can exploit well-developed engineering techniques to analyze the stability of truss-like structures.²⁰ Specifically, overall tractions are imposed on the boundary of the network and the stability analysis is reduced to a well-defined linear algebra problem. If the network does not deform under these boundary conditions, then it is stable, or, equivalently, the packing is strictly jammed. If the network deforms, then the packing is not strictly jammed. To our knowledge, the use of such techniques to characterize jammed packings would be new.

The classification of random packings of d -dimensional spheres according to our criteria defined above possesses direct relevance to the ongoing search for maximally random jammed (MRJ) states. Even for a given choice of scalar order parameter ψ , the maximally random jammed state can be expected to depend nontrivially on which of the three jamming definitions (locally, collectively, or strictly jammed) has been imposed. It seems likely that there is a wide class of random packings that satisfy both the locally jammed and collectively

jammed criteria. However, it is not clear whether random packings can be strictly jammed with more than vanishingly small probability. In other words, it may be very unlikely to find collectively jammed configurations that are able to resist all shear deformations. As noted earlier, our suggested generalization of the rigidity percolation concept may prove valuable in identifying strictly jammed structures, and in characterizing those local geometric attributes which allow them to resist shear.

5 Concluding Remarks

We have shown that there is a multiplicity of generation, selection, and classification procedures for jammed configurations of identical d -dimensional hard spheres. In particular, we have given three different definitions for jammed configurations: (1) locally jammed configuration; (2) collectively jammed configuration; and (3) strictly jammed configuration. Importantly, the particular classification of a random packing depends crucially on the type of boundary conditions imposed as well as the shape of the boundary. We also have shown how the concept of rigidity percolation, previously applied to understand the mechanical properties of network glasses, can be generalized to characterize hard-sphere packings even further. We have categorized common ordered lattices according to our definitions and discuss implications for random disk and sphere packings. Thus, we see that the characterization of jammed hard-particle packings is inherently nonunique and that the choice one makes is ultimately problem-dependent. Finally, we have discussed the practical implementation of our three different definitions for jammed configurations.

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Table 1: Classification of some of the common jammed ordered lattices of equi-sized spheres in two and three dimensions, where Z denotes the coordination number and ϕ is the packing fraction for the infinite lattice. Here hard boundaries are applicable: in two dimensions we use commensurate rectangular boundaries and in three dimensions we use a cubical boundary, with the exception of the hexagonal close-packed lattice in which the natural choice is a hexagonal prism.

Lattice	Locally jammed	Collectively jammed	Strictly jammed
Honeycomb ($Z = 3$, $\phi \approx 0.605$)	yes	no	no
Kagomé ($Z = 4$, $\phi \approx 0.680$)	no ^a	no ^a	no ^a
Square ($Z = 4$, $\phi \approx 0.785$)	yes	yes	no
Triangular ($Z = 6$, $\phi \approx 0.907$)	yes	yes	yes
Diamond ($Z = 4$, $\phi \approx 0.340$)	yes	no	no
Simple cubic ($Z = 6$, $\phi \approx 0.524$)	yes	yes	no
Body-centered cubic ($Z = 8$, $\phi \approx 0.680$)	yes	yes	no
Face-centered cubic ($Z = 12$, $\phi \approx 0.741$)	yes	yes	yes
Hexagonal close-packed ($Z = 12$, $\phi \approx 0.741$)	yes	yes	yes

^aWith appropriately placed regular triangular- or hexagonal-shaped boundaries, the Kagomé lattice is locally, collectively and strictly jammed.

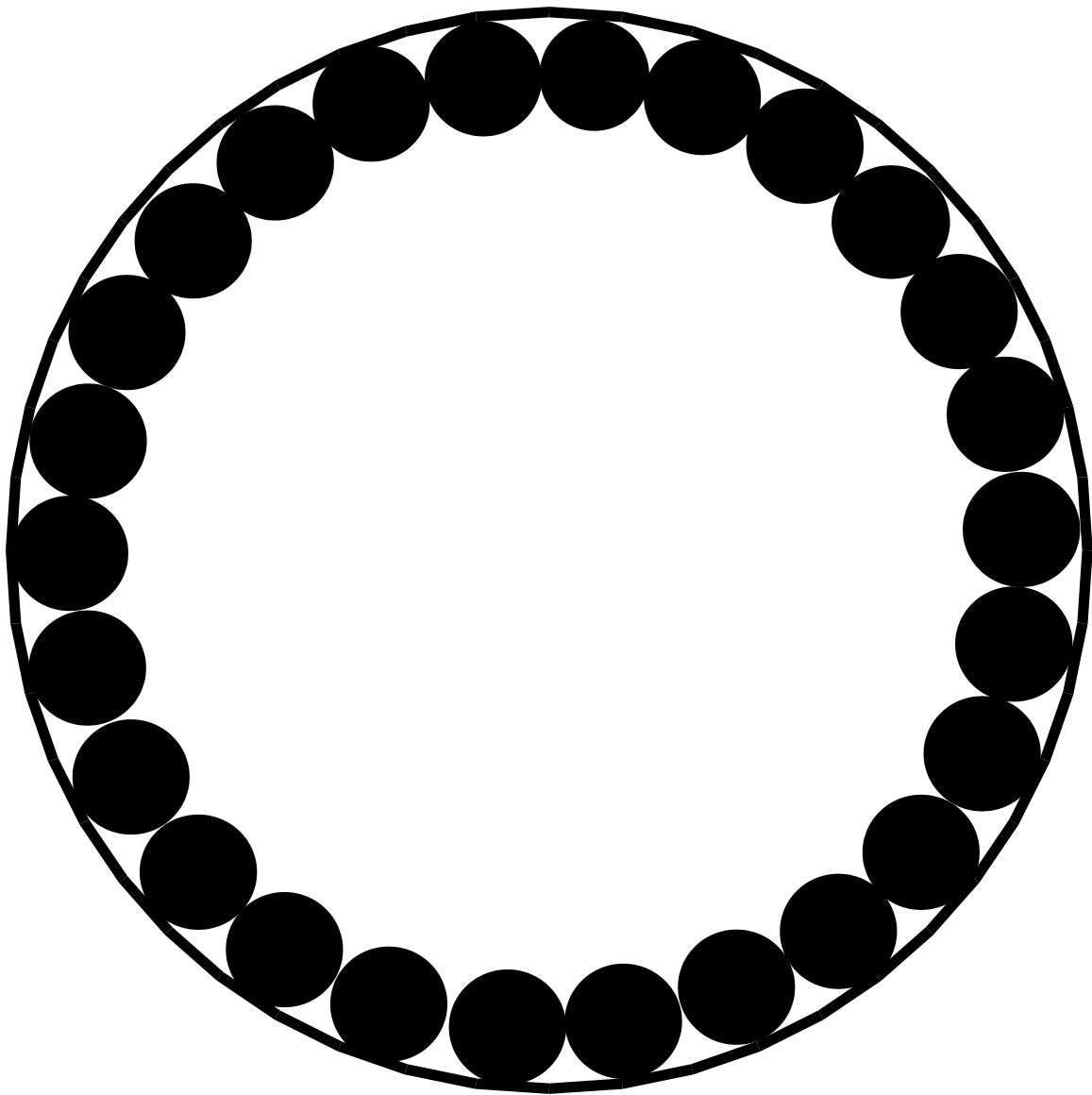


Figure 1: A jammed system in which all of the particles are in contact with the boundary.

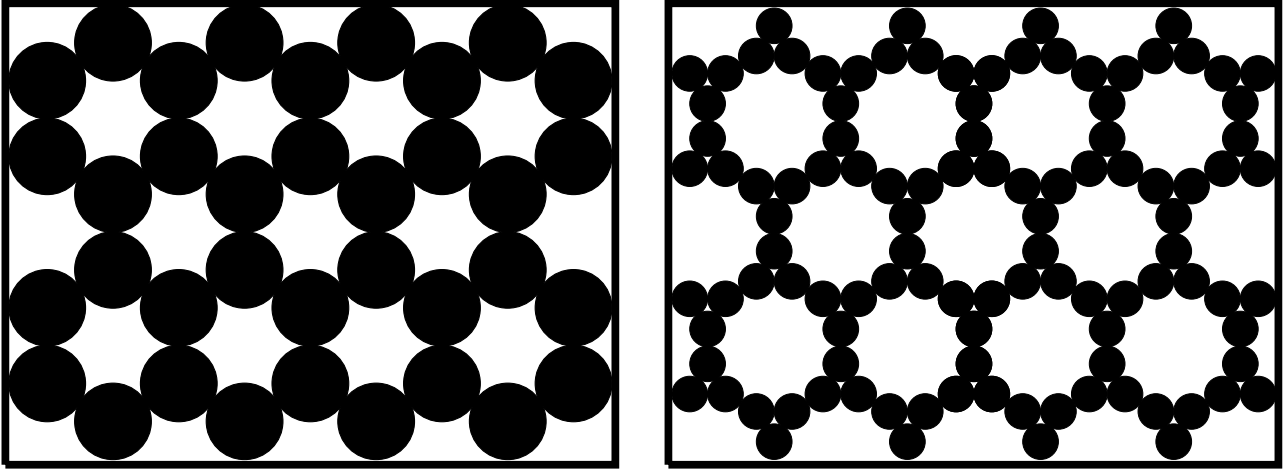


Figure 2: Left panel: The honeycomb (hexagonal) lattice can be made locally jammed but not collectively jammed with a hard rectangular boundary. Right panel: The packing that results by placing within each disk in the left panel three smaller disks that are locally jammed and then removing the larger disks. This procedure is a means of creating low-density jammed structures in the infinite-volume limit.

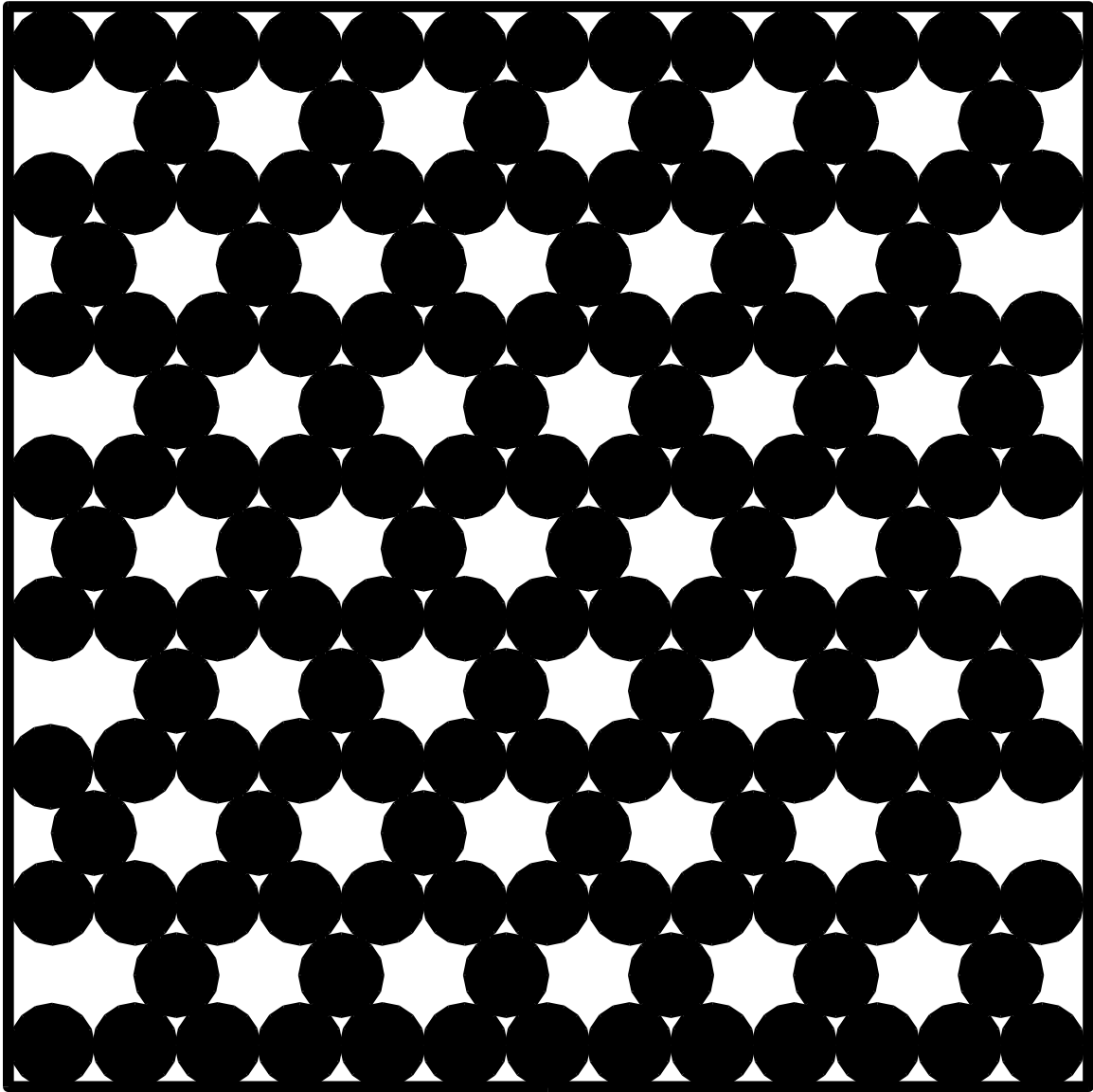


Figure 3: The Kagomé lattice is not locally jammed with a hard rectangular boundary. However, when properly situated within a container with a regular triangular- or hexagonal-shaped boundary, it can be made to be strictly jammed.

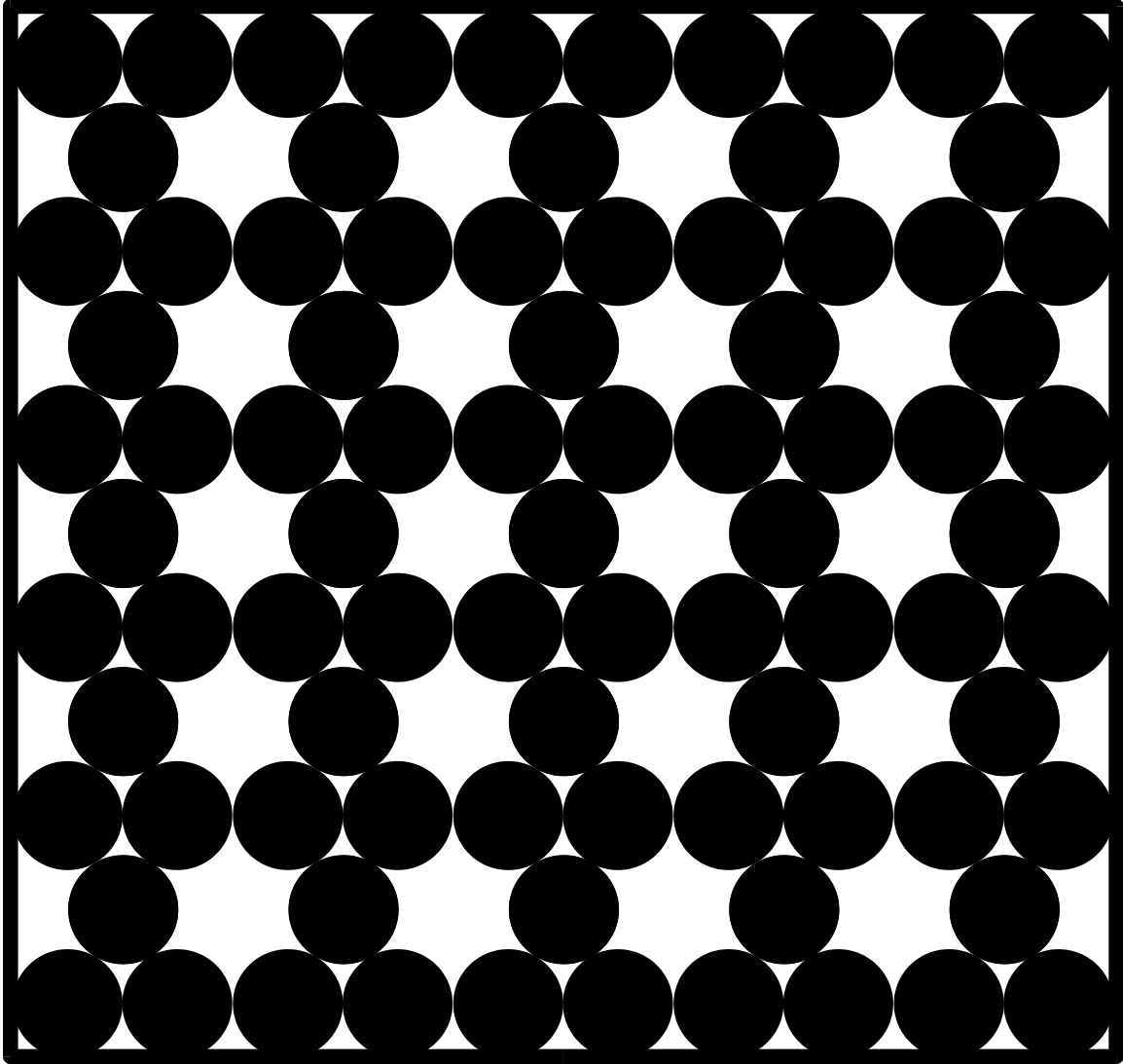


Figure 4: An example of a two-dimensional packing that is collectively jammed with a hard rectangular boundary.